



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2016 – 12:57 PM EDT

PDB ID : 5FMO
Title : Crystal structure and proteomics analysis of empty virus like particles of Cowpea mosaic virus
Authors : Huynh, N.; Hesketh, E.L.; Saxena, P.; Meshcheriakova, Y.; Ku, Y.C.; Hoang, L.; Johnson, J.E.; Ranson, N.A.; Lomonosoff, G.P.; Reddy, V.S.
Deposited on : 2015-11-07
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

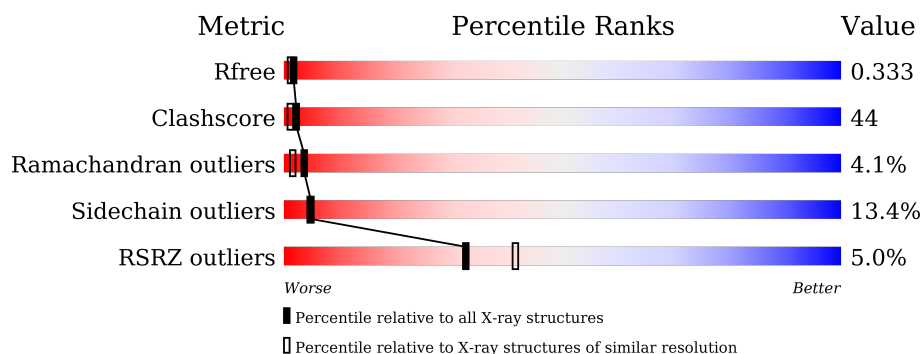
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	374	<div> <div>5%</div> <div> <div></div> <div>39%</div> <div>51%</div> <div>9%</div> </div> </div>
2	S	213	<div> <div>5%</div> <div> <div></div> <div>36%</div> <div>46%</div> <div>8%</div> <div>9%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4440 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called EMPTY VIRUS LIKE PARTICLES OF COWPEA MOSAIC VIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	370	Total	C	N	O	S	0	0	1
			2866	1822	481	541	22			

- Molecule 2 is a protein called EMPTY VIRUS LIKE PARTICLES OF COWPEA MOSAIC VIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	194	Total	C	N	O	S	0	0	1
			1516	971	256	280	9			

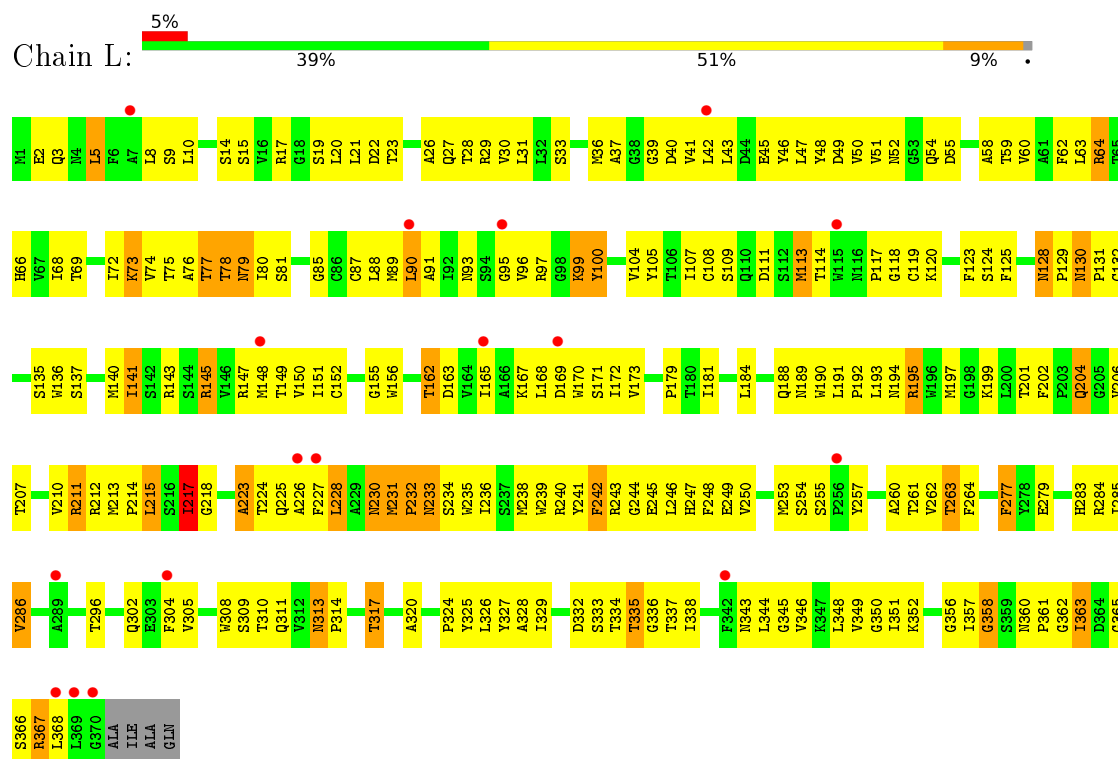
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	45	Total	O	0	0
			45	45		
3	S	13	Total	O	0	0
			13	13		

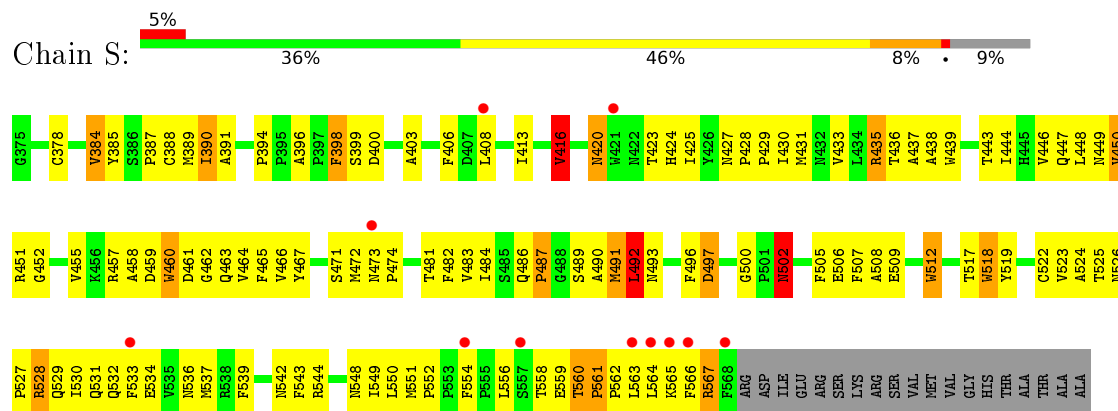
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: EMPTY VIRUS LIKE PARTICLES OF COWPEA MOSAIC VIRUS



• Molecule 2: EMPTY VIRUS LIKE PARTICLES OF COWPEA MOSAIC VIRUS



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	655.97Å 655.97Å 571.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30 49.95 – 2.30	Depositor EDS
% Data completeness (in resolution range)	58.3 (10.00-2.30) 60.2 (49.95-2.30)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.29Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.359 , 0.362 0.334 , 0.333	Depositor DCC
R_{free} test set	96064 reflections (3.10%)	DCC
Wilson B-factor (Å ²)	7.7	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.11 , 132.8	EDS
Estimated twinning fraction	0.105 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.15$	Xtriage
Outliers	0 of 3192363 reflections	Xtriage
F_o, F_c correlation	0.54	EDS
Total number of atoms	4440	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	L	0.44	0/2933	0.70	1/3985 (0.0%)
2	S	0.52	0/1564	0.79	3/2143 (0.1%)
All	All	0.47	0/4497	0.73	4/6128 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	384	VAL	CB-CA-C	-10.30	91.82	111.40
2	S	561	PRO	CB-CA-C	-5.18	99.06	112.00
1	L	361	PRO	CB-CA-C	-5.10	99.24	112.00
2	S	492	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2866	0	2813	265	0
2	S	1516	0	1456	135	0
3	L	45	0	0	20	0
3	S	13	0	0	7	0
All	All	4440	0	4269	384	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 44.

All (384) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:22:ASP:O	1:L:58:ALA:HB2	1.60	1.01
2:S:466:VAL:CG2	2:S:482:PHE:HB2	2.03	0.89
1:L:96:VAL:HG12	2:S:550:LEU:HB2	1.55	0.87
1:L:37:ALA:O	1:L:155:GLY:N	2.07	0.87
2:S:447:GLN:HG3	2:S:493:ASN:HD21	1.40	0.86
1:L:263:THR:HB	1:L:285:ILE:HD13	1.57	0.86
1:L:30:VAL:HG22	1:L:43:LEU:HD13	1.55	0.86
3:L:2018:HOH:O	2:S:502:ASN:HB3	1.75	0.86
2:S:566:PHE:O	2:S:567:ARG:HB2	1.77	0.85
1:L:313:ASN:HD22	1:L:314:PRO:N	1.76	0.83
2:S:398:PHE:HE1	2:S:400:ASP:HB2	1.43	0.82
1:L:313:ASN:HA	1:L:363:ILE:HD11	1.62	0.82
2:S:466:VAL:HG23	2:S:482:PHE:HB2	1.61	0.81
2:S:484:ILE:O	2:S:484:ILE:HD12	1.81	0.81
1:L:36:MET:O	1:L:155:GLY:HA2	1.80	0.81
1:L:36:MET:HB2	1:L:40:ASP:OD2	1.81	0.80
1:L:120:LYS:NZ	3:L:2016:HOH:O	2.11	0.79
2:S:450:VAL:HG23	2:S:490:ALA:H	1.47	0.79
1:L:343:ASN:HB2	3:L:2034:HOH:O	1.82	0.78
1:L:199:LYS:HE2	1:L:343:ASN:ND2	1.98	0.78
1:L:2:GLU:HG2	1:L:3:GLN:N	1.97	0.78
1:L:199:LYS:HE2	1:L:343:ASN:HD22	1.49	0.77
2:S:428:PRO:HD2	2:S:431:MET:HB2	1.67	0.77
1:L:26:ALA:HB3	1:L:170:TRP:HB2	1.65	0.76
2:S:528:ARG:HA	2:S:528:ARG:NH1	2.00	0.76
2:S:463:GLN:HB2	2:S:525:THR:OG1	1.86	0.75
1:L:59:THR:O	1:L:62:PHE:HB3	1.87	0.75
2:S:447:GLN:HG3	2:S:493:ASN:ND2	2.02	0.74
1:L:305:VAL:HG23	3:L:2043:HOH:O	1.88	0.74
1:L:218:GLY:HA3	1:L:311:GLN:HB3	1.71	0.72
1:L:253:MET:HG3	3:L:2033:HOH:O	1.88	0.72
2:S:465:PHE:HB2	2:S:523:VAL:CG1	2.20	0.72
1:L:228:LEU:H	1:L:228:LEU:HD12	1.53	0.72
1:L:75:THR:HA	1:L:124:SER:HB3	1.71	0.72
1:L:141:ILE:H	1:L:141:ILE:HD13	1.55	0.71
1:L:140:MET:HA	2:S:512:TRP:CZ3	2.24	0.71
1:L:230:ASN:HD21	1:L:233:ASN:HB3	1.55	0.71
2:S:471:SER:HA	2:S:519:TYR:CE2	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:23:THR:HG22	1:L:171:SER:HB3	1.71	0.70
2:S:471:SER:HA	2:S:519:TYR:HE2	1.56	0.70
1:L:215:LEU:HD23	1:L:325:TYR:HA	1.75	0.69
1:L:277:PHE:N	1:L:277:PHE:HD1	1.89	0.69
1:L:217:ILE:HD13	1:L:217:ILE:H	1.58	0.69
1:L:277:PHE:CD1	1:L:277:PHE:N	2.59	0.68
1:L:223:ALA:HB3	1:L:226:ALA:O	1.94	0.68
1:L:235:TRP:O	1:L:238:MET:HG2	1.94	0.68
1:L:261:THR:HB	1:L:332:ASP:OD1	1.94	0.68
1:L:93:ASN:HD22	2:S:548:ASN:HD22	1.41	0.68
2:S:450:VAL:O	2:S:489:SER:HB2	1.94	0.68
1:L:210:VAL:C	1:L:211:ARG:HD2	2.14	0.68
1:L:113:MET:HE1	1:L:124:SER:HA	1.76	0.67
1:L:113:MET:HE3	1:L:125:PHE:HD1	1.58	0.67
2:S:403:ALA:HB2	2:S:523:VAL:HG23	1.76	0.67
2:S:524:ALA:HB1	2:S:530:ILE:HD12	1.77	0.66
2:S:560:THR:C	2:S:562:PRO:HD2	2.16	0.66
1:L:93:ASN:ND2	2:S:548:ASN:HD22	1.92	0.66
2:S:428:PRO:HD2	2:S:431:MET:CB	2.25	0.66
1:L:33:SER:H	1:L:36:MET:CE	2.08	0.66
1:L:113:MET:HE3	1:L:125:PHE:CD1	2.31	0.65
1:L:47:LEU:O	1:L:50:VAL:HG12	1.97	0.65
1:L:231:MET:HB3	1:L:232:PRO:HD3	1.79	0.65
1:L:230:ASN:HD21	1:L:233:ASN:CB	2.09	0.65
2:S:481:THR:HA	3:S:2007:HOH:O	1.97	0.65
1:L:113:MET:CE	1:L:125:PHE:HD1	2.10	0.64
1:L:37:ALA:HA	1:L:155:GLY:HA3	1.79	0.64
2:S:486:GLN:HG3	2:S:490:ALA:HB2	1.78	0.64
1:L:48:TYR:O	1:L:51:VAL:HG22	1.98	0.64
1:L:42:LEU:HD21	1:L:152:CYS:HB2	1.79	0.64
1:L:99:LYS:O	2:S:552:PRO:HB3	1.97	0.64
1:L:230:ASN:ND2	1:L:233:ASN:HB3	2.11	0.64
2:S:388:CYS:HB3	2:S:431:MET:SD	2.37	0.64
1:L:162:THR:HG22	1:L:163:ASP:H	1.63	0.63
1:L:313:ASN:C	1:L:313:ASN:HD22	2.02	0.63
2:S:385:TYR:C	3:S:2003:HOH:O	2.36	0.63
1:L:206:VAL:O	1:L:206:VAL:HG12	1.98	0.63
1:L:225:GLN:HA	1:L:225:GLN:NE2	2.14	0.63
1:L:46:TYR:N	1:L:147:ARG:HH11	1.95	0.63
1:L:225:GLN:HA	1:L:225:GLN:HE21	1.63	0.63
1:L:214:PRO:HA	1:L:325:TYR:CE1	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:443:THR:HG23	2:S:542:ASN:HD21	1.64	0.63
1:L:260:ALA:HB2	1:L:334:THR:HA	1.81	0.63
2:S:465:PHE:HB2	2:S:523:VAL:HG12	1.81	0.63
1:L:36:MET:HG3	1:L:36:MET:O	1.99	0.62
2:S:563:LEU:O	2:S:565:LYS:HG2	1.99	0.62
1:L:230:ASN:HD22	1:L:230:ASN:C	2.01	0.62
1:L:45:GLU:HA	1:L:147:ARG:NH1	2.14	0.62
1:L:74:VAL:HA	3:L:2007:HOH:O	1.98	0.62
1:L:15:SER:OG	1:L:69:THR:HG22	1.99	0.62
1:L:193:LEU:HD11	1:L:351:ILE:HG12	1.81	0.62
1:L:313:ASN:HD22	1:L:314:PRO:CD	2.13	0.62
2:S:448:LEU:HB3	2:S:492:LEU:CD1	2.30	0.62
2:S:430:ILE:O	2:S:433:VAL:HG22	1.99	0.61
1:L:217:ILE:N	1:L:217:ILE:HD13	2.16	0.61
2:S:563:LEU:O	2:S:565:LYS:N	2.34	0.61
2:S:389:MET:HE2	2:S:406:PHE:HD1	1.65	0.60
1:L:72:ILE:HD11	1:L:136:TRP:CZ2	2.36	0.60
1:L:23:THR:CG2	1:L:172:ILE:H	2.14	0.60
2:S:450:VAL:HG12	2:S:533:PHE:CD1	2.36	0.60
1:L:130:ASN:HD22	1:L:130:ASN:C	2.02	0.60
1:L:141:ILE:N	1:L:141:ILE:HD13	2.16	0.60
1:L:329:ILE:N	1:L:329:ILE:HD12	2.15	0.60
2:S:528:ARG:CZ	2:S:528:ARG:HA	2.31	0.60
1:L:313:ASN:ND2	1:L:314:PRO:HD2	2.17	0.60
1:L:5:LEU:H	1:L:5:LEU:HD12	1.66	0.60
2:S:509:GLU:HG3	2:S:517:THR:HB	1.84	0.59
2:S:560:THR:N	2:S:561:PRO:CD	2.66	0.59
1:L:227:PHE:CD2	1:L:365:GLY:HA2	2.38	0.59
1:L:45:GLU:C	1:L:147:ARG:HH11	2.06	0.59
2:S:500:GLY:HA3	2:S:505:PHE:C	2.22	0.59
1:L:217:ILE:CD1	1:L:217:ILE:H	2.15	0.59
1:L:80:ILE:HG23	1:L:118:GLY:HA2	1.85	0.59
1:L:195:ARG:HD3	1:L:233:ASN:OD1	2.03	0.59
1:L:46:TYR:HB2	1:L:49:ASP:OD2	2.03	0.59
1:L:135:SER:HA	3:L:2006:HOH:O	2.01	0.59
1:L:80:ILE:HD12	1:L:81:SER:H	1.67	0.59
2:S:492:LEU:O	2:S:492:LEU:HD13	2.02	0.59
1:L:245:GLU:HB3	1:L:352:LYS:HB3	1.84	0.58
1:L:190:TRP:HE1	1:L:192:PRO:HG3	1.67	0.58
2:S:559:GLU:HB3	2:S:561:PRO:HD2	1.86	0.58
2:S:451:ARG:HD2	2:S:532:GLN:OE1	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:344:LEU:HA	3:L:2033:HOH:O	2.04	0.58
1:L:304:PHE:HB2	3:L:2030:HOH:O	2.04	0.57
1:L:231:MET:HE1	1:L:232:PRO:HA	1.86	0.57
1:L:63:LEU:H	1:L:63:LEU:HD22	1.69	0.57
1:L:28:THR:HG21	1:L:50:VAL:HG23	1.85	0.57
2:S:517:THR:HG23	2:S:518:TRP:N	2.18	0.57
2:S:566:PHE:O	2:S:567:ARG:CB	2.51	0.57
1:L:181:ILE:N	1:L:181:ILE:HD12	2.19	0.56
2:S:464:VAL:HB	2:S:484:ILE:HD11	1.87	0.56
1:L:137:SER:O	1:L:140:MET:HB3	2.05	0.56
1:L:253:MET:N	3:L:2033:HOH:O	2.36	0.56
2:S:561:PRO:O	2:S:562:PRO:C	2.39	0.56
1:L:190:TRP:NE1	1:L:192:PRO:HG3	2.21	0.56
1:L:233:ASN:O	1:L:236:ILE:HG22	2.06	0.56
1:L:88:LEU:CD2	1:L:117:PRO:HD3	2.36	0.56
1:L:21:LEU:O	1:L:21:LEU:HD23	2.05	0.56
1:L:104:VAL:HG13	1:L:105:TYR:N	2.20	0.56
1:L:23:THR:CG2	1:L:172:ILE:N	2.69	0.56
2:S:460:TRP:HA	2:S:529:GLN:HE22	1.69	0.56
1:L:193:LEU:HD12	1:L:350:GLY:HA2	1.88	0.56
1:L:213:MET:O	1:L:325:TYR:HD1	1.88	0.55
1:L:149:THR:HG22	1:L:150:VAL:N	2.21	0.55
1:L:357:ILE:HD12	1:L:357:ILE:N	2.22	0.55
2:S:452:GLY:HA2	2:S:531:GLN:H	1.71	0.55
1:L:263:THR:HB	1:L:285:ILE:CD1	2.31	0.55
1:L:76:ALA:HA	1:L:167:LYS:O	2.07	0.55
1:L:87:CYS:HB2	1:L:253:MET:HB3	1.87	0.55
1:L:113:MET:CE	1:L:124:SER:HA	2.36	0.55
2:S:389:MET:HG2	2:S:425:ILE:HD12	1.89	0.55
2:S:455:VAL:HG11	2:S:529:GLN:HE21	1.71	0.55
1:L:225:GLN:HA	2:S:556:LEU:HD12	1.89	0.54
1:L:109:SER:HB3	1:L:230:ASN:OD1	2.07	0.54
1:L:90:LEU:HD22	1:L:150:VAL:HG22	1.89	0.54
1:L:42:LEU:HB2	1:L:150:VAL:HG12	1.87	0.54
2:S:448:LEU:HD23	2:S:449:ASN:N	2.23	0.54
2:S:398:PHE:CE1	2:S:400:ASP:HB2	2.34	0.54
2:S:465:PHE:O	2:S:523:VAL:HG12	2.08	0.54
1:L:349:VAL:N	3:L:2031:HOH:O	2.38	0.54
1:L:33:SER:H	1:L:36:MET:HE1	1.72	0.54
2:S:431:MET:O	2:S:435:ARG:HD3	2.07	0.54
2:S:466:VAL:C	2:S:467:TYR:HD1	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:394:PRO:HA	2:S:420:ASN:O	2.07	0.53
1:L:233:ASN:C	1:L:233:ASN:HD22	2.12	0.53
2:S:389:MET:HB3	2:S:413:ILE:HD11	1.90	0.53
1:L:365:GLY:O	1:L:366:SER:HB3	2.09	0.53
1:L:63:LEU:N	1:L:63:LEU:HD22	2.24	0.53
2:S:528:ARG:NH1	3:S:2004:HOH:O	2.41	0.53
1:L:145:ARG:HH11	1:L:145:ARG:HB2	1.73	0.53
1:L:108:CYS:O	1:L:194:ASN:HB3	2.09	0.52
1:L:332:ASP:CG	1:L:333:SER:H	2.12	0.52
2:S:430:ILE:HG13	2:S:539:PHE:CE2	2.44	0.52
1:L:149:THR:HG22	1:L:150:VAL:H	1.75	0.52
1:L:45:GLU:CA	1:L:147:ARG:HH11	2.23	0.52
1:L:313:ASN:HA	1:L:363:ILE:CD1	2.38	0.52
2:S:561:PRO:N	2:S:562:PRO:CD	2.72	0.52
2:S:460:TRP:HA	2:S:529:GLN:NE2	2.25	0.52
1:L:249:GLU:N	3:L:2032:HOH:O	2.42	0.52
1:L:28:THR:CG2	1:L:50:VAL:HG23	2.39	0.52
1:L:89:MET:CE	1:L:91:ALA:HB2	2.40	0.52
1:L:72:ILE:HD13	1:L:129:PRO:HD3	1.92	0.51
1:L:95:GLY:O	2:S:549:ILE:HA	2.10	0.51
1:L:43:LEU:C	1:L:43:LEU:HD23	2.31	0.51
1:L:349:VAL:HB	3:L:2031:HOH:O	2.11	0.51
1:L:33:SER:N	1:L:36:MET:CE	2.73	0.51
1:L:73:LYS:HD3	1:L:75:THR:OG1	2.10	0.51
1:L:362:GLY:HA3	2:S:429:PRO:HD3	1.93	0.51
1:L:45:GLU:HA	1:L:147:ARG:HH11	1.76	0.51
1:L:239:TRP:O	1:L:310:THR:HG21	2.10	0.51
1:L:68:ILE:HD13	1:L:137:SER:HA	1.91	0.51
1:L:211:ARG:N	1:L:211:ARG:HD2	2.25	0.50
1:L:193:LEU:HD21	1:L:236:ILE:HD12	1.93	0.50
1:L:85:GLY:N	1:L:255:SER:HB2	2.26	0.50
2:S:438:ALA:HB2	2:S:549:ILE:HG23	1.93	0.50
1:L:2:GLU:HG2	1:L:3:GLN:H	1.75	0.50
1:L:197:MET:HB2	1:L:346:VAL:O	2.11	0.50
2:S:443:THR:HG22	2:S:497:ASP:CG	2.31	0.50
1:L:254:SER:N	3:L:2034:HOH:O	2.44	0.50
1:L:313:ASN:ND2	1:L:314:PRO:CD	2.75	0.50
1:L:72:ILE:HD12	1:L:72:ILE:N	2.27	0.50
1:L:23:THR:HG22	1:L:172:ILE:H	1.77	0.50
1:L:248:PHE:CE1	1:L:348:LEU:HB2	2.47	0.50
2:S:396:ALA:HA	3:S:2004:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:214:PRO:HA	1:L:325:TYR:CD1	2.47	0.49
1:L:36:MET:O	1:L:36:MET:CG	2.61	0.49
1:L:141:ILE:H	1:L:141:ILE:CD1	2.22	0.49
2:S:389:MET:HG2	2:S:425:ILE:CD1	2.42	0.49
1:L:231:MET:HE2	1:L:231:MET:C	2.34	0.49
1:L:231:MET:HB2	2:S:436:THR:O	2.13	0.49
1:L:64:ARG:N	1:L:64:ARG:HD2	2.28	0.48
1:L:68:ILE:HG21	1:L:136:TRP:CZ2	2.48	0.48
1:L:88:LEU:HD22	1:L:88:LEU:N	2.28	0.48
2:S:448:LEU:HB3	2:S:492:LEU:HD13	1.95	0.48
1:L:128:ASN:HD22	1:L:129:PRO:HD2	1.77	0.48
1:L:212:ARG:HH11	1:L:212:ARG:HG3	1.78	0.48
2:S:450:VAL:HG12	2:S:533:PHE:HD1	1.76	0.48
1:L:113:MET:CE	1:L:125:PHE:CD1	2.92	0.48
1:L:143:ARG:C	1:L:145:ARG:H	2.15	0.48
1:L:167:LYS:C	1:L:168:LEU:HD22	2.33	0.48
2:S:544:ARG:HG3	2:S:544:ARG:HH11	1.79	0.48
1:L:128:ASN:C	1:L:128:ASN:HD22	2.16	0.48
1:L:89:MET:HE2	1:L:91:ALA:HB2	1.96	0.48
2:S:435:ARG:HD3	2:S:435:ARG:H	1.79	0.48
1:L:169:ASP:C	3:L:2007:HOH:O	2.52	0.47
1:L:335:THR:OG1	1:L:336:GLY:N	2.47	0.47
2:S:462:GLY:O	2:S:463:GLN:HG3	2.13	0.47
2:S:465:PHE:HB3	2:S:467:TYR:HE1	1.78	0.47
2:S:387:PRO:O	2:S:428:PRO:HG2	2.15	0.47
1:L:211:ARG:HH11	1:L:211:ARG:HG2	1.79	0.47
1:L:50:VAL:HG21	1:L:170:TRP:NE1	2.30	0.47
2:S:496:PHE:N	2:S:496:PHE:CD1	2.83	0.47
2:S:506:GLU:C	3:S:2006:HOH:O	2.52	0.47
1:L:195:ARG:HG3	1:L:195:ARG:O	2.13	0.47
1:L:233:ASN:C	1:L:233:ASN:ND2	2.68	0.47
1:L:239:TRP:C	1:L:360:ASN:HB2	2.34	0.47
1:L:179:PRO:HB2	1:L:181:ILE:CD1	2.45	0.47
2:S:430:ILE:HD13	2:S:537:MET:O	2.14	0.47
2:S:443:THR:HG22	2:S:497:ASP:OD2	2.14	0.47
1:L:59:THR:O	1:L:63:LEU:CD2	2.63	0.47
2:S:408:LEU:HB3	2:S:537:MET:HE1	1.97	0.47
1:L:128:ASN:HD22	1:L:129:PRO:CD	2.28	0.47
2:S:403:ALA:O	2:S:416:VAL:HG22	2.15	0.47
1:L:184:LEU:HD11	2:S:543:PHE:HB3	1.96	0.47
1:L:284:ARG:HG3	1:L:284:ARG:HH11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:29:ARG:HG3	1:L:29:ARG:NH1	2.31	0.46
2:S:500:GLY:HA3	2:S:505:PHE:O	2.14	0.46
1:L:250:VAL:HG13	1:L:346:VAL:HG22	1.97	0.46
2:S:413:ILE:HG13	2:S:425:ILE:HD11	1.98	0.46
1:L:246:LEU:HD13	1:L:351:ILE:HD12	1.98	0.46
1:L:73:LYS:HB2	1:L:173:VAL:CG1	2.46	0.46
2:S:406:PHE:O	2:S:519:TYR:HA	2.16	0.46
2:S:537:MET:N	3:S:2003:HOH:O	2.47	0.46
1:L:262:VAL:O	1:L:286:VAL:HG23	2.15	0.46
1:L:75:THR:HG23	1:L:124:SER:HB3	1.96	0.46
1:L:193:LEU:HD12	1:L:193:LEU:N	2.30	0.46
1:L:88:LEU:HD23	1:L:117:PRO:HD3	1.98	0.46
1:L:162:THR:HG22	1:L:163:ASP:N	2.30	0.46
1:L:367:ARG:H	1:L:367:ARG:HG2	1.51	0.46
2:S:561:PRO:N	2:S:562:PRO:HD2	2.31	0.46
2:S:551:MET:HB3	2:S:552:PRO:HD2	1.98	0.46
2:S:493:ASN:N	2:S:493:ASN:HD22	2.14	0.45
2:S:450:VAL:HG12	2:S:533:PHE:CE1	2.51	0.45
1:L:73:LYS:HB2	1:L:173:VAL:HG13	1.98	0.45
1:L:226:ALA:HB1	2:S:554:PHE:O	2.16	0.45
1:L:247:HIS:O	1:L:348:LEU:HD12	2.16	0.45
1:L:311:GLN:CD	1:L:363:ILE:CG2	2.85	0.45
3:L:2018:HOH:O	2:S:505:PHE:HB2	2.17	0.45
1:L:337:THR:O	1:L:338:ILE:HD13	2.16	0.45
2:S:390:ILE:HG22	2:S:424:HIS:HB2	1.98	0.45
1:L:132:CYS:HA	1:L:181:ILE:HD11	1.99	0.45
1:L:42:LEU:HD22	1:L:42:LEU:H	1.82	0.45
2:S:448:LEU:CD1	2:S:466:VAL:HG11	2.47	0.45
1:L:23:THR:HG23	1:L:172:ILE:H	1.82	0.45
1:L:311:GLN:OE1	1:L:363:ILE:HG22	2.17	0.45
1:L:362:GLY:CA	2:S:429:PRO:HD3	2.47	0.45
2:S:471:SER:OG	2:S:473:ASN:ND2	2.50	0.45
1:L:97:ARG:HB3	2:S:551:MET:CE	2.47	0.45
1:L:148:MET:HE3	1:L:170:TRP:CZ2	2.51	0.45
1:L:90:LEU:HD21	1:L:148:MET:HE1	1.98	0.45
1:L:317:THR:HG23	1:L:320:ALA:HB3	1.98	0.44
1:L:8:LEU:C	1:L:10:LEU:H	2.18	0.44
1:L:367:ARG:HE	1:L:367:ARG:HB3	1.64	0.44
1:L:128:ASN:ND2	1:L:128:ASN:C	2.70	0.44
1:L:23:THR:HG22	1:L:172:ILE:N	2.32	0.44
1:L:241:TYR:HD1	1:L:309:SER:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:260:ALA:CB	1:L:334:THR:HA	2.46	0.44
1:L:223:ALA:N	1:L:368:LEU:HD13	2.32	0.44
2:S:389:MET:HE2	2:S:413:ILE:HG12	2.00	0.44
2:S:449:ASN:HB2	2:S:534:GLU:HB3	2.00	0.44
1:L:130:ASN:C	1:L:130:ASN:ND2	2.71	0.43
1:L:231:MET:HG3	2:S:437:ALA:HA	2.00	0.43
1:L:327:TYR:HB3	1:L:329:ILE:CD1	2.48	0.43
1:L:356:GLY:C	1:L:357:ILE:HD12	2.37	0.43
2:S:427:ASN:N	2:S:428:PRO:HD3	2.32	0.43
1:L:137:SER:O	1:L:141:ILE:CD1	2.66	0.43
1:L:29:ARG:HG3	1:L:29:ARG:HH11	1.83	0.43
1:L:225:GLN:HE21	1:L:225:GLN:CA	2.25	0.43
1:L:36:MET:O	1:L:155:GLY:CA	2.59	0.43
1:L:96:VAL:HB	1:L:100:TYR:CD2	2.54	0.43
2:S:450:VAL:O	2:S:489:SER:CB	2.65	0.43
2:S:457:ARG:O	2:S:459:ASP:N	2.51	0.43
2:S:559:GLU:C	2:S:561:PRO:HD2	2.39	0.43
1:L:244:GLY:O	1:L:246:LEU:HD22	2.19	0.43
1:L:89:MET:HE1	1:L:107:ILE:HG13	2.00	0.43
1:L:90:LEU:HD21	1:L:148:MET:CE	2.47	0.43
2:S:465:PHE:CE1	2:S:483:VAL:HG23	2.54	0.43
1:L:327:TYR:HB3	1:L:329:ILE:HD11	2.01	0.43
1:L:66:HIS:O	1:L:137:SER:HB3	2.18	0.43
2:S:413:ILE:HG21	2:S:423:THR:HG22	2.00	0.43
2:S:484:ILE:C	2:S:484:ILE:HD12	2.37	0.43
1:L:254:SER:HB3	3:L:2034:HOH:O	2.18	0.43
2:S:464:VAL:HB	2:S:484:ILE:CD1	2.49	0.43
1:L:77:THR:O	1:L:78:THR:HB	2.18	0.43
2:S:460:TRP:CD2	2:S:487:PRO:HA	2.53	0.43
2:S:466:VAL:HG12	2:S:522:CYS:SG	2.59	0.43
2:S:387:PRO:HA	2:S:536:ASN:OD1	2.19	0.43
1:L:326:LEU:HD23	1:L:327:TYR:N	2.34	0.43
1:L:85:GLY:HA3	1:L:255:SER:N	2.34	0.43
1:L:2:GLU:CG	1:L:3:GLN:N	2.77	0.42
1:L:328:ALA:C	1:L:329:ILE:HD12	2.39	0.42
1:L:129:PRO:O	1:L:131:PRO:HD3	2.19	0.42
1:L:255:SER:C	1:L:257:TYR:H	2.21	0.42
1:L:248:PHE:HE1	1:L:348:LEU:HB2	1.82	0.42
2:S:465:PHE:HB3	2:S:467:TYR:CE1	2.54	0.42
1:L:55:ASP:O	1:L:55:ASP:OD1	2.38	0.42
1:L:62:PHE:CD2	1:L:63:LEU:HD13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:439:TRP:HA	3:S:2006:HOH:O	2.19	0.42
1:L:100:TYR:O	1:L:100:TYR:HD1	2.02	0.42
1:L:255:SER:C	1:L:257:TYR:N	2.73	0.42
1:L:42:LEU:HD23	1:L:151:ILE:C	2.40	0.42
1:L:79:ASN:HA	1:L:79:ASN:HD22	1.62	0.42
1:L:95:GLY:HA3	2:S:549:ILE:HG22	2.02	0.42
2:S:528:ARG:NH1	2:S:528:ARG:CA	2.78	0.42
1:L:130:ASN:HA	1:L:131:PRO:HD2	1.88	0.42
1:L:225:GLN:O	1:L:226:ALA:HB2	2.19	0.42
1:L:264:PHE:N	1:L:264:PHE:CD1	2.86	0.42
1:L:250:VAL:HA	1:L:345:GLY:O	2.19	0.42
1:L:130:ASN:ND2	1:L:132:CYS:H	2.18	0.42
2:S:394:PRO:HG3	2:S:398:PHE:CD2	2.55	0.42
2:S:398:PHE:CD1	2:S:398:PHE:C	2.92	0.42
1:L:357:ILE:O	1:L:358:GLY:O	2.38	0.42
2:S:472:MET:HG2	2:S:519:TYR:CE2	2.54	0.42
1:L:263:THR:CB	1:L:285:ILE:HD13	2.38	0.42
1:L:360:ASN:ND2	1:L:362:GLY:HA2	2.35	0.42
1:L:63:LEU:H	1:L:63:LEU:CD2	2.31	0.42
1:L:168:LEU:HD22	1:L:168:LEU:N	2.35	0.41
1:L:20:LEU:HD23	1:L:20:LEU:O	2.20	0.41
1:L:264:PHE:O	1:L:283:HIS:HB2	2.20	0.41
1:L:27:GLN:HA	1:L:168:LEU:O	2.20	0.41
1:L:242:PHE:HE1	1:L:308:TRP:NE1	2.18	0.41
1:L:333:SER:HA	3:L:2028:HOH:O	2.20	0.41
2:S:430:ILE:HG23	2:S:431:MET:H	1.84	0.41
2:S:560:THR:N	2:S:561:PRO:HD3	2.35	0.41
1:L:201:THR:HA	3:L:2027:HOH:O	2.19	0.41
1:L:243:ARG:NH2	3:L:2030:HOH:O	2.54	0.41
1:L:78:THR:O	1:L:78:THR:HG23	2.20	0.41
2:S:403:ALA:HB2	2:S:523:VAL:CG2	2.46	0.41
2:S:394:PRO:CA	2:S:420:ASN:O	2.67	0.41
1:L:230:ASN:HD21	1:L:233:ASN:H	1.68	0.41
1:L:368:LEU:O	1:L:368:LEU:HG	2.20	0.41
2:S:561:PRO:C	2:S:562:PRO:O	2.55	0.41
1:L:43:LEU:HD23	1:L:43:LEU:O	2.20	0.41
1:L:59:THR:O	1:L:63:LEU:HD22	2.20	0.41
1:L:218:GLY:CA	1:L:311:GLN:HB3	2.43	0.41
1:L:41:VAL:O	1:L:41:VAL:HG13	2.20	0.41
1:L:19:SER:C	1:L:21:LEU:H	2.24	0.41
1:L:95:GLY:CA	2:S:549:ILE:HG22	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:8:LEU:O	1:L:10:LEU:N	2.45	0.41
2:S:449:ASN:ND2	2:S:491:MET:HE3	2.36	0.41
1:L:107:ILE:HD11	1:L:151:ILE:HD13	2.02	0.41
2:S:390:ILE:HD13	2:S:391:ALA:N	2.36	0.41
2:S:398:PHE:HD1	2:S:399:SER:N	2.19	0.41
1:L:202:PHE:HB3	1:L:334:THR:HG21	2.03	0.41
1:L:204:GLN:HA	1:L:334:THR:OG1	2.21	0.40
1:L:80:ILE:CG2	1:L:118:GLY:HA2	2.51	0.40
1:L:365:GLY:O	1:L:366:SER:CB	2.68	0.40
1:L:85:GLY:O	1:L:156:TRP:HA	2.22	0.40
2:S:526:ASN:OD1	2:S:528:ARG:HB3	2.21	0.40
1:L:23:THR:HG23	1:L:172:ILE:O	2.21	0.40
1:L:46:TYR:N	1:L:147:ARG:NH1	2.66	0.40
2:S:444:ILE:HB	2:S:496:PHE:CE1	2.56	0.40
2:S:446:VAL:HG12	2:S:447:GLN:N	2.37	0.40
2:S:400:ASP:O	2:S:527:PRO:HG3	2.21	0.40
1:L:230:ASN:O	1:L:234:SER:HB2	2.21	0.40
2:S:447:GLN:CG	2:S:493:ASN:HD21	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	368/374 (98%)	301 (82%)	54 (15%)	13 (4%)	4	2
2	S	192/213 (90%)	164 (85%)	18 (9%)	10 (5%)	2	1
All	All	560/587 (95%)	465 (83%)	72 (13%)	23 (4%)	3	1

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	39	GLY
1	L	54	GLN
2	S	458	ALA
2	S	567	ARG
1	L	217	ILE
1	L	279	GLU
1	L	358	GLY
1	L	363	ILE
2	S	564	LEU
1	L	78	THR
1	L	99	LYS
1	L	223	ALA
2	S	474	PRO
2	S	502	ASN
2	S	512	TRP
1	L	9	SER
1	L	52	ASN
1	L	232	PRO
1	L	324	PRO
2	S	508	ALA
2	S	416	VAL
2	S	487	PRO
2	S	560	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	318/320 (99%)	271 (85%)	47 (15%)	4	3
2	S	167/183 (91%)	149 (89%)	18 (11%)	8	9
All	All	485/503 (96%)	420 (87%)	65 (13%)	5	5

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5	LEU

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Mol	Chain	Res	Type
1	L	14	SER
1	L	17	ARG
1	L	31	LEU
1	L	60	VAL
1	L	64	ARG
1	L	73	LYS
1	L	77	THR
1	L	79	ASN
1	L	90	LEU
1	L	100	TYR
1	L	111	ASP
1	L	113	MET
1	L	114	THR
1	L	119	CYS
1	L	123	PHE
1	L	128	ASN
1	L	130	ASN
1	L	141	ILE
1	L	145	ARG
1	L	162	THR
1	L	165	ILE
1	L	188	GLN
1	L	189	ASN
1	L	191	LEU
1	L	195	ARG
1	L	204	GLN
1	L	207	THR
1	L	211	ARG
1	L	215	LEU
1	L	217	ILE
1	L	224	THR
1	L	228	LEU
1	L	230	ASN
1	L	231	MET
1	L	233	ASN
1	L	240	ARG
1	L	242	PHE
1	L	263	THR
1	L	277	PHE
1	L	286	VAL
1	L	296	THR
1	L	302	GLN

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Mol	Chain	Res	Type
1	L	313	ASN
1	L	317	THR
1	L	335	THR
1	L	367	ARG
2	S	378	CYS
2	S	384	VAL
2	S	390	ILE
2	S	398	PHE
2	S	416	VAL
2	S	420	ASN
2	S	435	ARG
2	S	450	VAL
2	S	460	TRP
2	S	461	ASP
2	S	491	MET
2	S	492	LEU
2	S	497	ASP
2	S	502	ASN
2	S	507	PHE
2	S	518	TRP
2	S	528	ARG
2	S	558	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	3	GLN
1	L	52	ASN
1	L	79	ASN
1	L	93	ASN
1	L	128	ASN
1	L	130	ASN
1	L	188	GLN
1	L	204	GLN
1	L	225	GLN
1	L	230	ASN
1	L	311	GLN
1	L	313	ASN
1	L	343	ASN
1	L	360	ASN
2	S	447	GLN
2	S	470	GLN

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Mol	Chain	Res	Type
2	S	473	ASN
2	S	486	GLN
2	S	493	ASN
2	S	502	ASN
2	S	529	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	L	370/374 (98%)	0.21	17 (4%) 36 45	33, 69, 97, 159	0
2	S	194/213 (91%)	0.38	11 (5%) 27 36	39, 74, 116, 188	0
All	All	564/587 (96%)	0.27	28 (4%) 32 41	33, 71, 102, 188	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	565	LYS	13.8
2	S	566	PHE	10.5
2	S	564	LEU	8.0
2	S	563	LEU	6.6
1	L	42	LEU	5.1
1	L	226	ALA	4.6
1	L	95	GLY	4.2
1	L	148	MET	3.7
1	L	370	GLY	3.3
1	L	115	TRP	3.0
1	L	342	PHE	3.0
1	L	304	PHE	3.0
2	S	421	TRP	2.9
1	L	369	LEU	2.9
1	L	227	PHE	2.8
2	S	568	PHE	2.8
1	L	169	ASP	2.8
2	S	408	LEU	2.7
1	L	7	ALA	2.6
2	S	533	PHE	2.6
1	L	165	ILE	2.5
1	L	368	LEU	2.4
2	S	554	PHE	2.4
2	S	473	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	289	ALA	2.1
1	L	256	PRO	2.1
2	S	557	SER	2.1
1	L	90	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.